AMENDMENTS TO THE CLAIMS:

Please amend claims 1 and 15, as set forth below.

This listing of claims will replace all prior versions and listings of claims in the Application:

Claim 1 (currently amended): A method of aligning a query protein sequence with a ~~template which comprises~~ a set of pre-selected protein structures in a database, to identify the structure ~~of the template~~ in the database that best fits the query protein sequence, comprising the steps of:

selecting an energy function, said energy function being a linear combination of energy parameters, with weight factors as coefficients;

establishing linear programming (LP) constraints for threading (or aligning) said query protein sequence with each structure in said set of pre-selected protein structures in a database; and

performing a linear programming analysis based on a linear programming formulation including said energy function under said constraints, to optimally align said query protein with said ~~template~~set of pre-selected protein structures, the structure of the template that optimally aligns with the query protein sequence being identified as the best fit.

Claim 2 (previously presented): The method of claim 1, further comprising the step of using training to determine values for said weight factors.

Claim 3 (original): The method of claim 2, where said energy function comprises the function: $min \ W_m E_m + W_s E_s + W_p E_p + W_g E_g + W_{ss} E_{ss}$.

Claim 4 (original): The method of claim 1, where alignment gaps are confined to loops.

4

Claim 5 (original): The method of claim 1, where only interaction between core residues is considered.

Claim 6 (previously presented): The method of claim 1, wherein said step of performing a linear programming analysis is done on the assumption that solutions are likely to be integral.

Claim 7 (original): The method of claim 6, wherein said step of performing a linear programming analysis comprises the step of using a branch and bound technique to perform said linear programming analysis.

Claim 8 (previously presented): The method of claim 1, where said linear programming constraints require that:

one core can be aligned to a unique sequence position;

conflicts between said core and the adjacent two cores are forbidden;

at most one interaction variable can have a value of 1 between any two cores that have interactions between each other;

if two cores have their alignments to the sequence respectively and also have interactions between them, then at least one interaction variable should be 1; and

the values of x (alignment variables) and y (interaction variables) are to be between 0 and 1 when the problem is relaxed to a linear program.

Claim 9 (previously presented): The method of claim 1, where said linear programming constraints require that:

one core can be aligned to a unique sequence position;

the values of x (alignment variables) and y (interaction variables) are to be between 0 and 1 when the problem is relaxed to a linear program;

conflicts between two neighbouring cores are forbidden; and

it is guaranteed that one interaction variable has a value of 1 if and only if its two

generating x variables have a value of 1.

Claim 10 (previously presented): The method of claim 1, where said linear programming

constraints require that:

one core can be aligned to a unique sequence position;

the values of x (alignment variables) and y (interaction variables) are to be between 0

and 1 when the problem is relaxed to a linear program; and

when one x variable is 1 is equivalent to that one of the y variables generated by it is 1.

Claim 11 (previously presented): The method of claim 1, further comprising the step of

performing graph reduction to decrease the number of integer variables and speed up the LP

analysis.

Claim 12 (canceled).

Claim 13 (original): The method of claim 1, comprising step of generating a dense contact

graph prior to said step of performing a linear programming analysis.

Claim 14 (canceled).

Claim 15 (currently amended): A system for aligning proteins comprising:

a computer operable to align a query protein sequence with a ~~template consisting of a~~

set of pre-selected protein structures in a database, to identify the structure ~~of the template~~ that

best fits the query protein sequence, by performing the steps of:

selecting an energy function;

determining values for weight factors in said energy function;

establishing linear programming (LP) constraints for threading (or aligning) said query

protein sequence with each structure in said set of pre-selected protein structures in a database;

and

performing a linear programming analysis based on a linear programming formulation

including said energy function under said constraints, to optimally align said query protein with

~~said template, the~~ each structure ~~of the template that optimally~~ in the database by linear

programming, the structure that aligns with the query protein sequence ~~being identified as the~~

~~best fit~~with the minimum energy score being the final output.